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Tungsten spectroscopy relevant to the diagnostics of ITER divertor plasmas

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Abstract

The possibility of using extreme ultraviolet emission from low charge states of tungsten ions to diagnose the divertor plasmas of the ITER tokamak has been investigated. Spectral modelling of Lu-like W^{3+} to Gd-like W^{10+} has been performed by using the Flexible Atomic Code, and spectroscopic measurements have been conducted at the Sustained Spheromak Physics Experiment (SSPX) in Livermore. To simulate ITER divertor plasmas, tungsten was introduced into the SSPX spheromak by prefilling it with tungsten hexacarbonyl prior to the usual hydrogen gas injection and initiation of the plasma discharge. The tungsten emission was studied using a grazing-incidence spectrometer.

1. Introduction

The divertor of the ITER tokamak will have tungsten target plates. Tungsten ions will sputter off the surfaces of the tiles at the particle strike points and get introduced into the plasma. The divertor plasmas will be relatively cool and have large temperature gradients. According to simulations by the ITER Physics Expert Group on Divertor [1], the electron temperatures will mainly be between 25 and 100 eV with peak temperatures around 150 eV close to the X point. Considering the ionization energies of tungsten, see [2] and table 1, and neglecting transport, a large fraction of the divertor plasmas can therefore be expected to contain tungsten ions in charge states mainly from three to ten times ionized.

The spectroscopic diagnostics considered for the ITER divertor include optical spectrometers and vacuum ultraviolet (VUV) spectrometers with wavelength coverage extending down in the soft x-ray region to 10 Å [3, 4]. As demonstrated in this paper, the 150–450 Å extreme ultraviolet (EUV) range may offer the best spectral region for monitoring of tungsten in the main divertor volume as the strong resonance lines of several low charge state tungsten ions fall in this region. However, it should be noted that plasma transport can add higher charge states of tungsten to the divertor that also could radiate in the EUV range, making the emission more complex, see e.g. [5]. Another advantage of the EUV interval is that expected low-*Z* impurities, such as carbon ions, offer strong *in situ* wavelength calibration lines, which could serve to measure carbon concentrations as well. The abundance of tungsten ions in the divertor is of importance for ITER operations as too large a quantity entering the confined core plasma could affect the plasma stability and ignition because of radiation losses. EUV tungsten spectra would be suitable to infer the concentrations and flow velocities and, given enough resolution, also could be used to measure ion temperatures in the divertor.

To assess where the strong line emission from low charge states of tungsten occurs, the structure and spectra of W^{3+}–W^{10+} have been calculated using the Flexible Atomic Code (FAC) [6]. The spectra have been modelled under magnetic fusion plasma conditions in the 100–1100 Å spectral range. Synthetic spectra of W^{5+}–W^{16+} in the 100–500 Å region have previously been presented by Peacock *et al* in their review of anticipated x-ray and VUV radiation in ITER [7].

Previously, the spectra of neutral to six times ionized tungsten have been studied [8, 9]. However, little focus has been given on the EUV range (150–450 Å) where, for charge states above four times ionized, strong resonance transitions are expected. The VUV spectrum of trebly ionized Lu-like W IV has been studied down to 673 Å by Iglesias *et al* [10] using a sliding-spark discharge. The spectrum of quadruply ionized tungsten, W V, isoelectronic to ytterbium, was first studied by Meijer using a sliding spark, leading to the identification of lines down to 638 Å [11]. Later studies by Kildiyarova *et al* [12] and Churilov *et al* [13], also using spark sources, observed lines down to 417 and 391 Å, respectively. The sixth spectrum of tungsten, Tm-like W VI, was also first investigated by Meijer [14] and later by Kaufman and Sugar [15, 16] resulting in wavelength measurements down to 382 Å. Sugar and Kaufman also observed Er-like W VII, again using

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Table 1. Tungsten ionization energies (IE). Excerpt from Kramida and Reader [2].

Ion	IE (eV)	Ion	IE (eV)
Neutral W	7.864	Ho-like W^{7+}	141.2
Ta-like W^{+}	16.37	Dy-like W^{8+}	160.2
Hf-like W^{2+}	26.0	Tb-like W^{9+}	179.0
Lu-like W^{3+}	38.2	Gd-like W^{10+}	208.9
Yb-like W^{4+}	51.6	Eu-like W^{11+}	231.6
Tm-like W^{5+}	64.77	Sm-like W^{12+}	258.2
Er-like W^{6+}	122.01	Pm-like W^{13+}	290.7

a sliding spark, and their measurement yielded wavelengths down to 130 Å [17]. Wyart *et al* re-examined those spectra and identified a number of lines in the 316–345 Å range [18]. A low-resolution observation of Ho-like W VIII in a tokamak plasma by Veres *et al*, indicated emission around 190 and 235 Å [19]. The spectra of higher charge states have, to our knowledge, not been investigated in any wavelength band until the tentative identification of 13 times ionized Pm-like W XIV, which Hutton *et al* may have observed at the Berlin electron-beam ion trap [20–22]. With the exception of Er-like W VII, low charge state tungsten spectra have not been studied in the EUV.

To simulate tungsten emission from ITER divertor plasmas, hydrogen discharges with trace amounts of tungsten have been produced at the Sustained Spheromak Physics Experiment facility (SSPX) at the Lawrence Livermore National Laboratory [23–25]. The SSPX spheromak, which was decommissioned in 2007, had plasma conditions comparable to those expected in the ITER divertor, with typical electron temperatures of around 100 eV and densities in the 10^{14-15} cm^{-3} range. The tungsten emission from SSPX plasmas can hence be assumed similar to those of the future ITER divertor or other magnetic fusion experiments operating in this low-temperature, high-density regime. The SSPX plasmas contained trace amounts of tungsten resulting from the usage of tungsten as a plasma-facing material coating the flux conserver. In addition to this intrinsic tungsten, a novel sublimation injector was constructed to increase the concentration of tungsten impurity ions in the spheromak plasmas. These tungsten-doped plasmas were studied spectroscopically using an $R = 5.6$ m grazing-incidence EUV spectrometer.

2. Spectral modelling

Based on ionization energies, the tungsten ions that can be expected to dominate the charge balance in the main plasma volume of the ITER divertor are Lu-like W^{3+} up to around Gd-like W^{10+}, see table 1. The spectra of these tungsten charge states have been calculated to guide the spheromak measurement and assess in which wavelength range the strong transitions occur. Some of these spectra have been studied experimentally in the past; however, those studies have been done at densities different from those found in magnetic fusion plasmas and, as such, line intensities can be quite different.

The calculations were performed using the Flexible Atomic Code, FAC v1.1.1., written by Gu [6]. The structure of the ions was calculated with closed K, L and M shells. Depending on spectral complexity, different numbers of energy levels and configuration interactions were included. Considered transitions comprise those involving ground configurations with valence electrons in $n = 5$, and excited configurations with one electron excited from the 4f subshell to $n = 5$ or 6, and electrons excited within the $n = 5$ shell or from $n = 5$ to $n = 6$. These multi-electron spectra are quite difficult to calculate with any accuracy because configuration-interaction effects are large, as noted by Sugar and Kaufman for Er-like W VII [17]. Comparisons with known line positions of W VII indicate that the calculated wavelengths are within 20 Å of the measured values. To aid the spectral analysis of the SSPX data, the low-Z impurity species were also calculated, i.e. carbon, nitrogen and oxygen. These systems were modelled with levels up to $n = 5$. Here, comparisons with known line positions listed by Kelly [26] show that most calculated line positions are within 10 Å of the experimental wavelengths.

The spectra were modelled at various electron temperatures and densities in order to have reference spectra from which to infer the SSPX temperatures. Spectra were calculated at densities of 10^{14} and 10^{15} cm^{-3}, but very little difference on the emission signatures was seen. However, as expected, the temperature had a strong effect and the spectra were therefore calculated in the 25–200 eV interval. The collisional-radiative spectral models include collisional excitation and de-excitation and autoionization. An overview of the calculated tungsten spectra is shown in figure 1 for $T_e = 100$ eV. It is clear that for charge states above four times ionized, Yb-like W V, the strong line radiation falls in the EUV region. It is also worth noting that the emissivities drop to very low values for ions above Ho-like W VIII, which means that for ITER divertor plasmas it is likely that only the very low charge states will be of interest for spectroscopic diagnostics. The spectra of Tm-like W VI, Er-like W VII and Ho-like W VIII are presented in greater detail in figure 2, where they are modelled in the 150–450 Å range at various temperatures with a resolution of $\Delta\lambda = 0.3$ Å full width at half-maximum (FWHM). The low-Z reference spectra at $T_e = 50$ eV are also presented, see figures 3–5. All presented spectra are calculated at $n_e = 10^{14}$ cm^{-3}.

3. Experimental setup

The tungsten study was performed at the SSPX spheromak facility, a small-size fusion experiment in Livermore [23–25]. The SSPX device produced self-organized toroidal plasmas lasting a few milliseconds. The tungsten was injected into the magnetically confined plasmas in the form of tungsten hexacarbonyl, $W(CO)_6$, a crystalline compound that also has been introduced into the Livermore SuperEBIT electron-beam ion trap for spectroscopic investigations of highly charged tungsten ions [27, 28]. Here, 5 g of tungsten hexacarbonyl was placed in a 1 l volume, which had been cleaned and purged with nitrogen gas. The volume and assembly were first

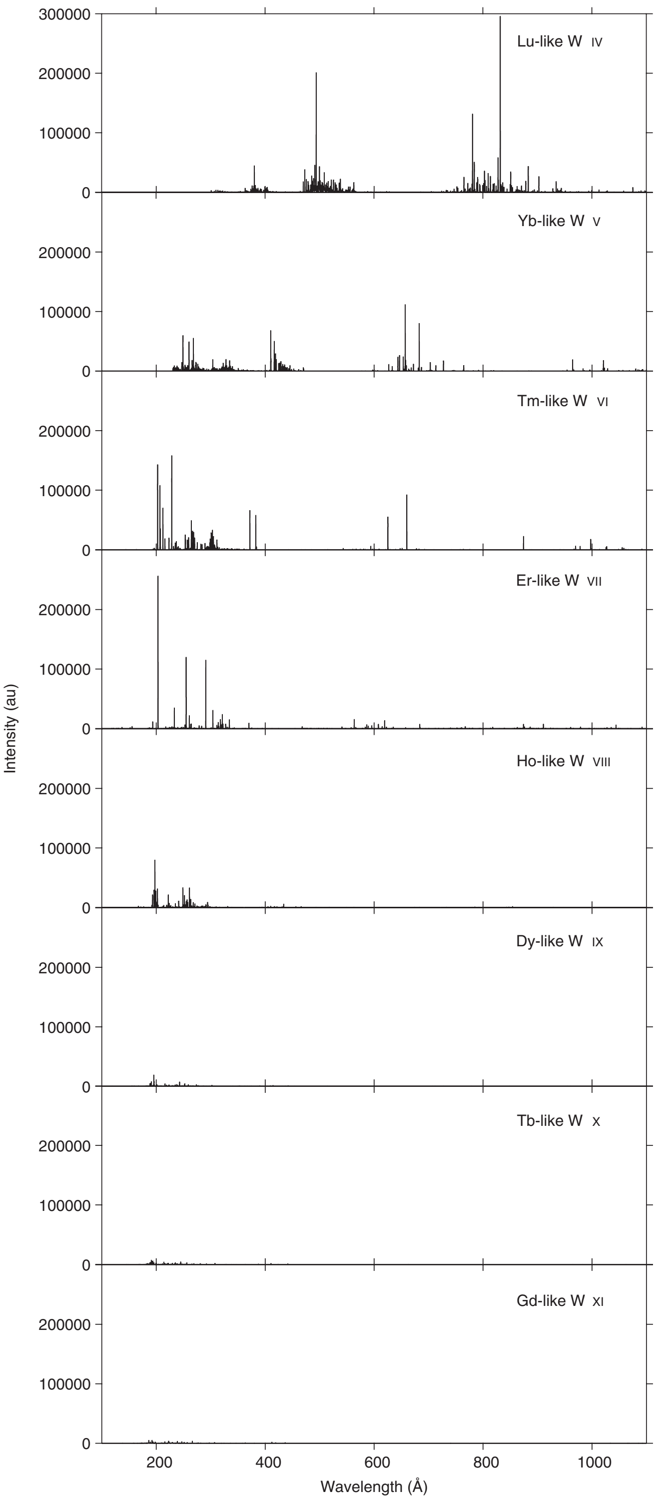

Figure 1. Calculated tungsten spectra at $T_e = 100$ eV and $n_e = 10^{14}$ cm^{-3}. The intensity scale is set to the same value for each charge state in order to provide a direct comparison of the expected line intensities.

evacuated to approximately 10^{-5} Torr and then heated using wrapped heater tapes. The pressure increase was monitored with a vacuum gauge and pressures were varied from 0.1 to 2 Torr by changing the temperature, which was recorded with a thermocouple. The tungsten-hexacarbonyl volume, which was connected to a view port of SSPX, was opened during the hydrogen prefill phase approximately 0.5 s prior to the discharge. As the tungsten gas pressures were higher than the SSPX vacuum-vessel pressure, the vapour could easily stream through a solenoid-controlled valve into the spheromak.

A high-resolution grazing-incidence spectrometer was used to study the tungsten emission. The same instrument has previously been used to study titanium and low-Z plasma impurities on SSPX [29–32] and is described in detail in [33]. For this experiment, the spectrometer was equipped with a Photometrics back-illuminated charge-coupled device (CCD) detector and a 30 μm entrance slit. With a field of view tangential to the magnetic axis of the spheromak, the observed emission originated from the cooler edge across to the hottest part at the centre of the plasma.

The spheromak plasmas were studied with and without tungsten injection to support the line-identification process. The toroidal plasma current was used to change the electron temperature. Record peak temperatures at SSPX have been noted to exceed 500 eV [24]; however, for this experiment the temperatures were likely in the 25–100 eV range. As the Thomson scattering electron-temperature diagnostic was offline, the plasma temperatures had to be inferred from the calculated spectra. The injection of tungsten into SSPX did not appear to have any negative effect on the spheromak performance, and plasma currents of up to around 1 MA were achieved during the few-millisecond discharges.

4. Analysis and results

Figures 6–8 show SSPX spectra in three regions where tungsten lines appear. The spectra were wavelength calibrated *in situ* using L-shell lines from carbon and oxygen. These lines, which also became enhanced during injection of tungsten hexacarbonyl, were observed in first and second orders. Spectra were also observed from helium, nitrogen, titanium and copper ions. The spectral lines were identified using the calculated spectra for line intensities and line lists from Kelly [26] for line positions. Even though the calculated wavelengths varied slightly from the measured positions, the intensities generally agreed well with the observed spectra. Lines that did not match any known spectra were likely candidates for being tungsten lines. Additionally, tungsten line identification was aided by the fact that the amounts of injected tungsten changed the observed spectra. Identified tungsten lines are listed in table 2, and unclassified candidate tungsten lines are listed in table 3.

The tungsten emission is dominated by Er-like W VII, which shows in most spectra. The Er-like W lines are identified based on the classifications by Sugar and Kaufman [17]. However, the line intensities given by Sugar and Kaufman do not agree with the observed SSPX intensities, which is likely due to the different densities of the emitting plasmas. For example, in Sugar and Kaufman's line list the strongest EUV line is the 261 Å line, which is six times stronger than the 216 Å line. In the SSPX spectra, the 216 Å line is generally the strongest line followed by the 261 Å line. Sugar and Kaufman list the 302 Å line and the 188 Å line to be about

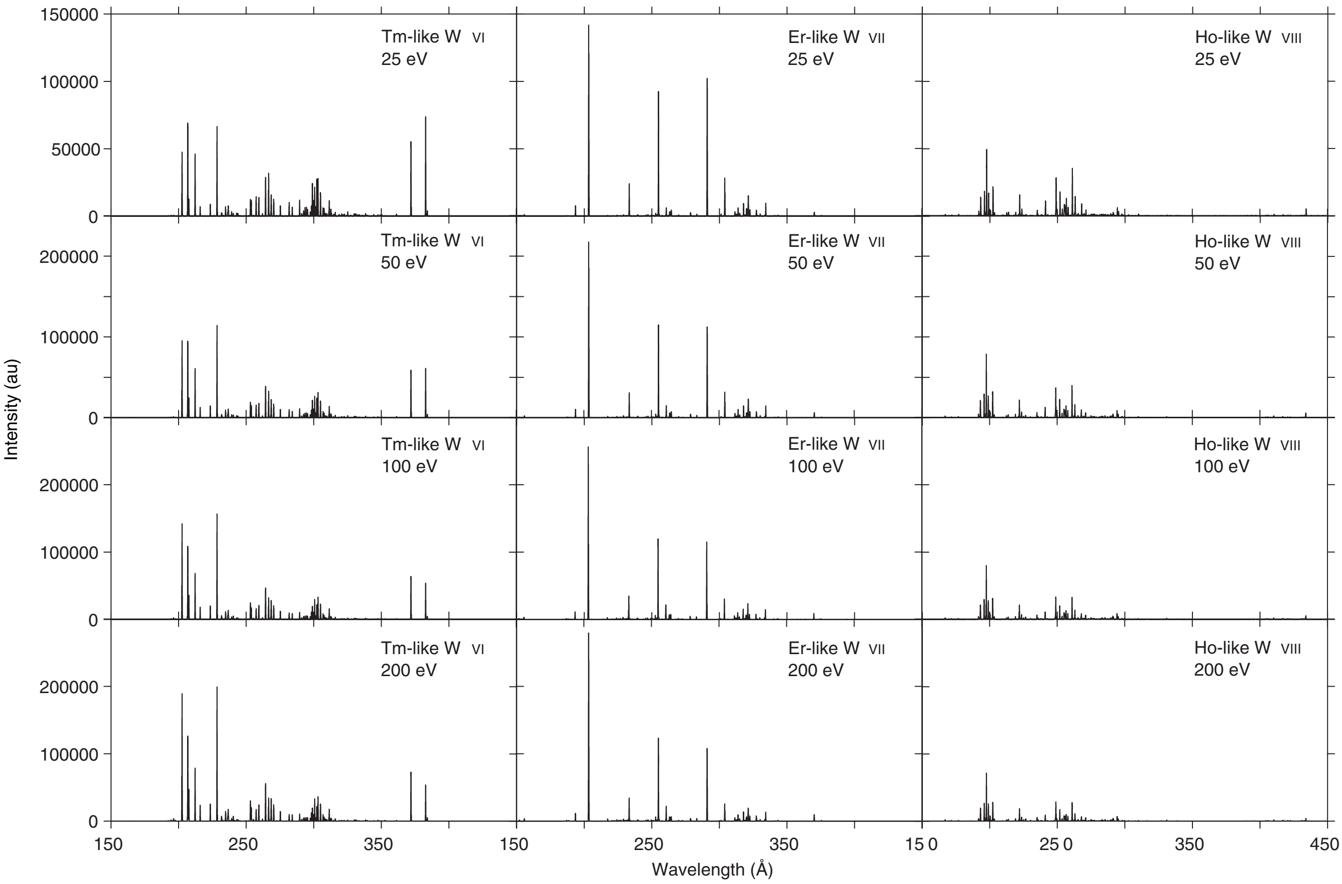

Figure 2. Calculated tungsten spectra at $n_e = 10^{14}$ cm^{-3} with $\Delta\lambda = 0.3$ Å FWHM. The spectra are labeled according to charge state and electron temperature.

Table 2. Observed tungsten lines in the SSPX spheromak.

Ion	Experiment λ (Å)	Prev. Exp. λ (Å)	Theory λ (Å)	Transition lower level	upper level
W^{6+}	188.15	188.159[a]	193.4	$(4f^{14}5s^25p^6)_0$	$(4f^{14}5s^25p_{1/2}5p^4_{3/2}6s_{1/2})_1$
W^{6+}	216.19	216.219[a]	203.2	$(4f^{14}5s^25p^6)_0$	$(4f^{14}5s^25p_{1/2}5p^4_{3/2}5d_{3/2})_1$
W^{6+}	223.82	223.846[a]	233.2	$(4f^{14}5s^25p^6)_0$	$(4f^{14}5s^25p^2_{1/2}5p^3_{3/2}6s_{1/2})_1$
W^{6+}	261.35	261.387[a]	254.9	$(4f^{14}5s^25p^6)_0$	$(4f^{14}5s^25p^2_{1/2}5p^3_{3/2}5d_{5/2})_1$
W^{6+}	289.44	289.526[a]	301.2	$(4f^{14}5s^25p^6)_0$	$(4f^5_{5/2}4f^8_{7/2}5s^25p^65d_{5/2})_1$
W^{6+}	294.37	294.376[a]	290.9	$(4f^{14}5s^25p^6)_0$	$(4f^5_{5/2}4f^8_{7/2}5s^25p^65d_{3/2})_1$
W^{6+}	302.28	302.272[a]	320.0	$(4f^{14}5s^25p^6)_0$	$(4f^6_{5/2}4f^7_{7/2}5s^25p^65d_{5/2})_1$
W^{6+}	313.64	313.573[a]	303.9	$(4f^{14}5s^25p^6)_0$	$(4f^{14}5s^25p^2_{1/2}5p^3_{3/2}5d_{3/2})_1$
W^{5+}	382.12	382.145[b]	371.9	$(4f^{14}5s^25p^65d_{3/2})_{3/2}$	$(4f^{14}5s^25p^65f_{5/2})_{5/2}$
W^{5+}	394.08	394.133[b]	382.7	$(4f^{14}5s^25p^65d_{5/2})_{5/2}$	$(4f^{14}5s^25p^65f_{7/2})_{7/2}$

[a] Sugar and Kaufman [17]
[b] Kaufman and Sugar [15, 16]

50 % more intense than the 216 line. Both these lines, however, are weaker in the SSPX spectra. The 289 Å line overlaps with a carbon line prohibiting a clear determination of its intensity, which according to the modelling should be very low. The 294 Å line is weaker and the 302 Å line much stronger than the calculations suggest. It is possible that the stronger intensity of the 302 Å line is due to a line blend. However, as noted earlier, these spectra are difficult to predict and even though Er-like W VII, with its closed-shell structure, should be the easiest to calculate, it is quite possible that the calculated spectra are not that accurate. The line at 313 Å is slightly off the value given by Sugar and Kaufman [17], which could mean that it is blended, too. Some of the lines identified by Wyart *et al* [18] possibly show around 330–340 Å as weak features.

Table 3. Candidate tungsten transitions in the SSPX spheromak.

Ion	Transition lower level	Upper level	Theory λ (Å)	Exp. candidate lines λ (Å)
W^{7+}	$(4f^{14}5s^25p_{1/2}^25p_{3/2}^3)_{3/2}$	$(4f^{14}5s^25p_{1/2}5p_{3/2}^35d_{3/2})_{3/2}$	193.2	194.5, 198.0, 198.8
W^{7+}	$(4f^{14}5s^25p_{1/2}^25p_{3/2}^3)_{3/2}$	$(4f^{14}5s^25p_{1/2}5p_{3/2}^35d_{3/2})_{1/2}$	195.9	198.0, 198.8, 200.5
W^{7+}	$(4f^{14}5s^25p_{1/2}^25p_{3/2}^3)_{3/2}$	$(4f^{14}5s^25p_{1/2}5p_{3/2}^35d_{3/2})_{5/2}$	197.5	201.8
W^{7+}	$(4f^{14}5s^25p_{1/2}5p_{3/2}^4)_{1/2}$	$(4f^{14}5s^25p_{3/2}^45d_{3/2})_{3/2}$	199.0	198.0, 198.8, 200.5, 205.3
W^{7+}	$(4f^{14}5s^25p_{1/2}^25p_{3/2}^3)_{3/2}$	$(4f^{14}5s^25p_{1/2}5p_{3/2}^35d_{3/2})_{3/2}$	202.3	200.5, 205.3, 208.0
W^{5+}	$(4f^{14}5s^25p^65d_{3/2})_{3/2}$	$(4f^{14}5s^25p_{1/2}5p_{3/2}^45d_{3/2}^2)_{3/2}$	202.5	198.0, 198.8, 200.5, 201.8, 205.3, 208.0
W^{5+}	$(4f^{14}5s^25p^65d_{5/2})_{5/2}$	$(4f^{14}5s^25p_{1/2}5p_{3/2}^45d_{3/2}5d_{5/2})_{5/2}$	206.7	205.3, 208.0, 211.0
W^{5+}	$(4f^{14}5s^25p^65d_{5/2})_{5/2}$	$(4f^{14}5s^25p_{1/2}5p_{3/2}^45d_{3/2}5d_{5/2})_{3/2}$	206.9	205.3, 208.0, 210.2, 211.0
W^{5+}	$(4f^{14}5s^25p^65d_{5/2})_{5/2}$	$(4f^{14}5s^25p_{1/2}5p_{3/2}^45d_{3/2}5d_{5/2})_{7/2}$	212.2	205.3, 208.0, 210.2, 211.0
W^{7+}	$(4f^{14}5s^25p_{1/2}5p_{3/2}^4)_{1/2}$	$(4f^{14}5s^25p_{1/2}5p_{3/2}^35d_{5/2})_{1/2}$	222.0	211.0, 218.4, 229.8
W^{5+}	$(4f^{14}5s^25p^65d_{3/2})_{3/2}$	$(4f^{14}5s^25p_{1/2}5p_{3/2}^45d_{3/2}^2)_{5/2}$	228.4	218.4, 229.8, 240.0, 241.8
W^{7+}	$(4f^{14}5s^25p_{1/2}^25p_{3/2}^3)_{3/2}$	$(4f^{14}5s^25p_{1/2}^25p_{3/2}^25d_{5/2})_{5/2}$	249.0	253.7, 254.3, 255.4, 259.3
W^{7+}	$(4f^{14}5s^25p_{1/2}^25p_{3/2}^3)_{3/2}$	$(4f^{14}5s^25p_{1/2}^25p_{3/2}^25d_{5/2})_{3/2}$	251.8	253.7, 254.3, 255.4, 259.3
W^{6+}	$(4f_{5/2}^54f_{7/2}^85s^25p^65d_{3/2})_1$	$(4f_{5/2}^54f_{7/2}^85s^25p^65f_{5/2})_0$	260.6	259.3, 276.2
W^{7+}	$(4f^{14}5s^25p_{1/2}^25p_{3/2}^3)_{3/2}$	$(4f_{5/2}^54f_{7/2}^85s^25p_{1/2}^25p_{3/2}^35d_{3/2})_{3/2}$	261.0	253.7, 254.3, 255.4, 259.3, 276.2
W^{7+}	$(4f^{14}5s^25p_{1/2}^25p_{3/2}^3)_{3/2}$	$(4f_{5/2}^64f_{7/2}^75s^25p_{1/2}^25p_{3/2}^35d_{5/2})_{5/2}$	263.1	253.7, 254.3, 255.4, 259.3, 276.2
W^{6+}	$(4f^{14}5s^25p_{1/2}^25p_{3/2}^35d_{5/2})_1$	$(4f^{14}5s^25p_{1/2}^25p_{3/2}^35f_{7/2})_2$	370.1	376.3

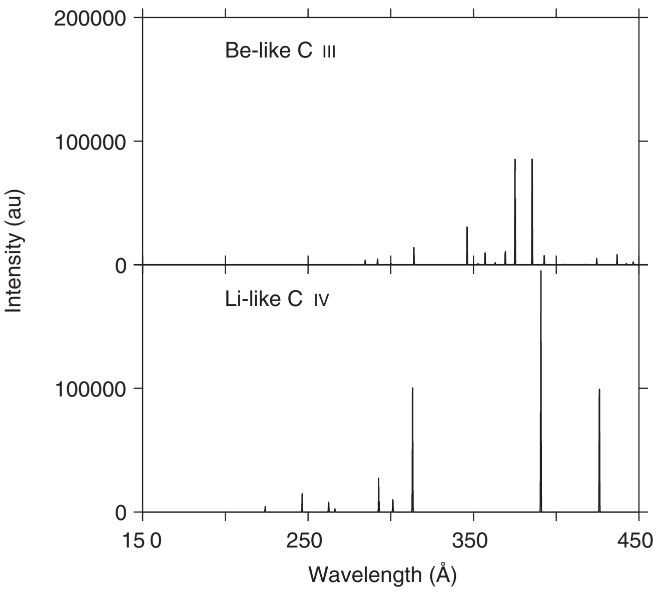

Figure 3. Calculated carbon spectra at $T_e = 50$ eV and $n_e = 10^{14}$ cm^{-3} with $\Delta\lambda = 0.3$ Å FWHM.

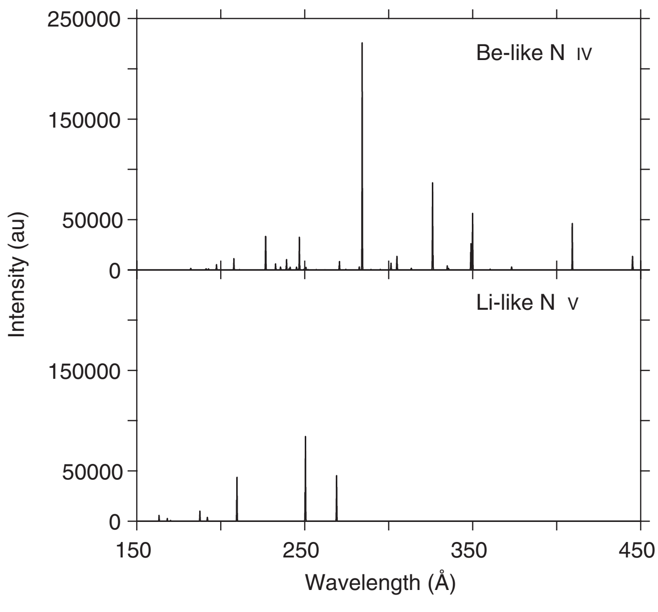

Figure 4. Calculated nitrogen spectra at $T_e = 50$ eV and $n_e = 10^{14}$ cm^{-3} with $\Delta\lambda = 0.3$ Å FWHM.

Based on the calculations, two groups of lines are believed to originate mainly from Ho-like W VIII. Ho-like W has previously been observed in a tokamak plasma at around 190 and 235 Å by Veres *et al* [19]. However, the features at around 202 and 255 Å in the SSPX spectra are shifted towards longer wavelengths relative to the tokamak spectrum. No reference lines were shown or discussed in [19], and a possible explanation of the shift could therefore be that their tokamak spectrometer had not been sufficiently calibrated.

Two 5d–5f transitions from Tm-like W VI are observed at 382 and 394 Å. Those are the shortest wavelengths previously measured in Tm-like W [15, 16]. The FAC calculations give several isolated Tm-like W lines in the EUV region, especially in the 200–240 Å range. These are not easy to identify, because there are plenty of lines in this region, including the Ho-like W candidate lines, and the calculations are not accurate enough to identify individual lines. The calculated

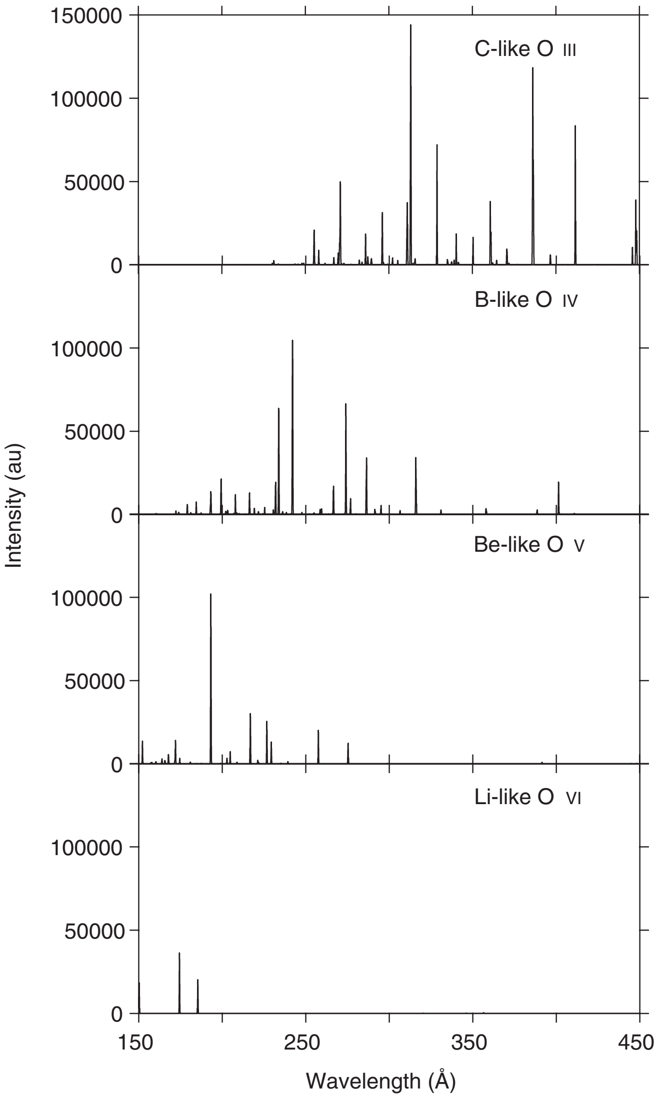

Figure 5. Calculated oxygen spectra at $T_e = 50$ eV and $n_e = 10^{14}$ cm^{-3} with $\Delta\lambda = 0.3$ Å FWHM.

lines can be both longer and shorter than the true line positions, and therefore the relative positions of the calculated lines may change. The Tm-like W candidate lines could be blended or interchanged with the Ho-like W candidate lines. Since many of the tungsten ions have several transitions around 200 Å, it is also possible that contributions from other charge states are blending with the candidate lines, in addition to the intrinsic impurity ions. Several tungsten candidate lines, however, have been identified. These lines are designated with red labels in the spectra. Based on the calculations, suggested candidate transitions are listed in table 3 with suggested line positions. Considering the agreement with the Er-like W lines, it is likely that the calculated wavelengths are within 20 Å of the actual values.

5. Summary

The tungsten emission from the SSPX plasmas is dominated by Er-like W VII with likely contributions from Tm-like W VI and Ho-like W VIII. The prevalence of Er-like W is due to the closed $4f^{14}5s^25p^6$ ground configuration, making the ion abundant over a large temperature interval and concentrating the emission into a few strong lines. The fact that Er-like W has strong isolated lines makes it very suitable for plasma diagnostics, especially to infer tungsten concentrations, ion temperatures and flow velocities.

However, even though the SSPX plasmas only show three charge states, it is quite possible that transport can affect the charge balance to look somewhat different in the ITER divertor. As indicated by the FAC calculations, the 150–450 Å spectral band contains strong emission from several charge states. Accurate atomic data on these ions will be necessary in order to realize tungsten spectroscopy in this wavelength regime as a viable divertor diagnostic. Although tungsten line positions can be determined from tungsten-doped plasmas, unambiguous line identifications can prove difficult as lines from neighbouring charge states often seem to be close and may even overlap, as our measurements have shown. In order to disentangle the emission and analyse relative line intensities, we are planning to extend this investigation at the Livermore low-energy electron-beam ion trap where there is more control over the ionization balance and the excitation processes [34, 35].

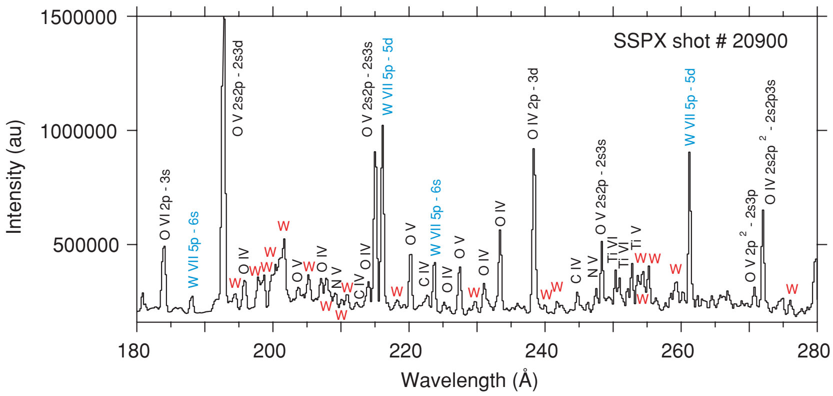

Figure 6. SSPX shot no. 20900. Low-temperature spheromak plasma with tungsten-hexacarbonyl injection. Tungsten lines are designated with blue labels and tungsten candidate lines with red labels. Also shown are lines from carbon, nitrogen, oxygen and titanium.

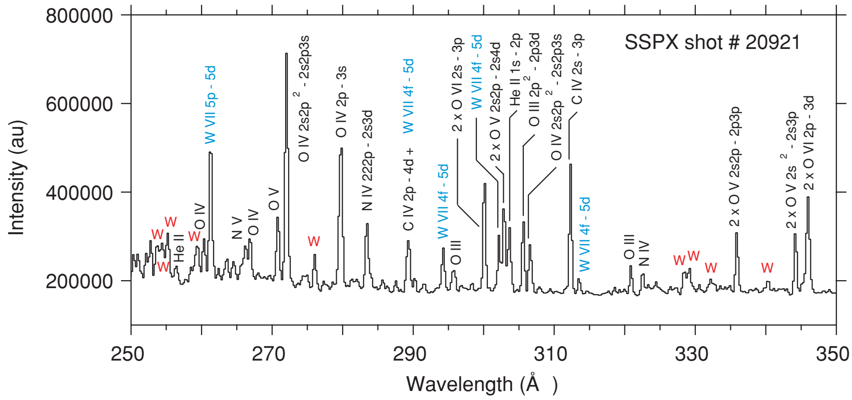

Figure 7. SSPX shot no. 20921. Low-temperature spheromak plasma with tungsten-hexacarbonyl injection. Tungsten lines are designated with blue labels and tungsten candidate lines with red labels. Also shown are lines from helium, carbon, nitrogen and oxygen.

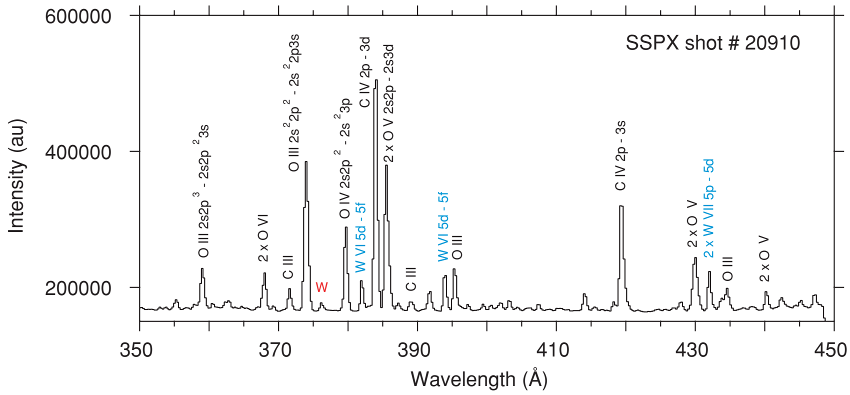

Figure 8. SSPX shot no. 20910. Low-temperature spheromak plasma with tungsten-hexacarbonyl injection. Tungsten lines are designated with blue labels and tungsten candidate lines with red labels. Also shown are lines from carbon, nitrogen and oxygen.

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